GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Fachbereich Physik
Institut für Theoretische Physik

CONDENSED MATTER THEORY SEMINAR

Subject: **From DFT to rBFM - Modelling structure formation of twin polymerization**

Speaker: **Janett Prehl (Technische Universität Chemnitz, Institut für Physik)**

Date & time: **Friday, October 28th, 2016 at 3:15 p.m.**

Venue: **Seminar room 1.114**

Due to the newly introduced method of twin polymerization [1], nanoporous hybrid materials containing organic and inorganic structure domains of 0.5 to 3 nm can be produced in a large variety of different compositions. Although first theoretical and experimental investigation have been performed, the open question still remains: How does the structure formation process of twin polymerization, yielding these interweaved organic-inorganic nanoporous hybrid materials, takes place in detail? Understanding the occurring effects and processes of the structure formation opens up the possibility to design (organic and/or inorganic) nanoporous materials with desired properties for industry. E.g. nanoporous materials are of great interest in applications like gas filter systems, catalyst or fuel cells.

After introducing the basic concepts of twin polymerization, I will show different modeling approaches for the complex reaction mechanism of twin polymerization. The utilized methods range from density functional theory (DFT) calculations [2] via reactive molecular dynamics simulation [3] to reactive Bond-Fluctuation-Models (rBFM). I will present and discuss obtained results and validate them with experimental results. Doing so insights to the structure formation process on different levels of length scale can be obtained.

References

[1] Grund, S., Kempe, P., Baumann, G., Seifert, A., and Spange, S. (2007) Zwillingspolymerisation: ein Weg zur Synthese von Nanokompositen. Angew. Chem., 119, 636-640.

[2] Tchernook, I., Prehl, J., and Friedrich, J. (2015) Quantum chemical investigation of the counter anion in the acid catalyzed initiation of 2,2'-spirobi[4H-1,3,2-benzodioxasiline] polymerization.
Polymer, 60, 241-251.

[3] Schönfelder, T., Friedrich, J., Prehl, J., Seeger, S., Spange, S., and Hoffmann, K. H. (2014) Reactive force field for electrophilic substitution at an aromatic system in twin polymerization.
Chem. Phys., 440, 119-126.